K18 Identification of Methcathinone in Urine by Gas Chromatography/Mass Spectrometry (GC/MS) Using a One-Step Simultaneous Dispersive Liquid-Liquid Extraction (LLE)/Cyclohexanone Derivatization

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After attending this presentation, attendees will have a better understanding of how cyclohexanone can be used as a simultaneous extraction and derivatizing agent.

This presentation will impact the forensic science community by providing a simple one-step dispersive (LLE)/derivatization method using GC/MS to identify methcathinone in urine.

Over the last decade, abuses of prescription and illegal drugs have caused serious problems in the United States. Recently a new class of drugs, known as synthetic cathinones, has spread worldwide. These synthetic cathinones are marketed as "bath salts," "legal high drugs," and "plant food." Synthetic cathinones are beta-ketone phenylalkylamine derivatives and are often termed "bk-amphetamines" for the beta-ketone moiety. One of the synthetic cathinones that has been abused illegally is methcathinone. Crime laboratories are in need of methods to detect and identify these drugs not only in solid-dosage form but also in biological fluids such as urine from suspects of driving under the influence.

Skymba and Brettell have previously investigated cyclohexanone as a derivatizing reagent for cathinones using GC/MS.[1] A method was developed using cyclohexanone to form the Schiff-base derivative, creating a more complicated mass spectrum and better separation of the synthetic cathinones. This GC/MS method was developed to screen, identify, and differentiate 11 similar cathinone compounds often present in illicit drug submissions to crime laboratories. Primary and secondary amines will react with cyclohexanone via a Schiff-base reaction to form two distinct, different types of derivatives. Cyclohexanone forms an imine derivative with primary amines and enamine derivatives with secondary amines. The method was found to be reproducible and can be used to screen unknown samples and identify multiple cathinones in one sample.

In this presentation, a method will be described which expands the role of the cyclohexanone to an extraction solvent as well as a derivatizing agent. The method uses 300uL of cyclohexanone as the extraction solvent in a one-step dispersive LLE/derivatization in which methcathinone can be detected and identified from 1mL of urine using GC/MS.

In this method, the GS oven temperature parameters were set with an initial temperature of 120ºC which then increased 15ºC/min to 275ºC. The column used was a 30m x 0.25mm x 0.25µm phenylmethylsilicone capillary column (Rxi®-5Sil MS) using helium as a carrier gas with a linear gas velocity of 36cm/sec. Cyclohexanone was used as the solvent and a sample volume of 1µL was injected in the split mode with a split ratio of 22:1. A retention-time optimization study provided the most advantageous separation conditions with methcathinone eluting with a retention time of 14.3 minutes using these conditions.

A simple, one-step dispersive LLE/derivatization method will be presented that uses cyclohexanone as the extraction solvent and GC/MS to identify methcathinone in urine.

Reference:

1. Brandi A. Skymba, M.S.F.S., and Thomas A. Brettell, Ph.D., "Investigation Into Cyclohexanone as a Schiff-Base Derivatizing Agent for the Detection of Cathinones with Gas Chromatography/Mass Spectrometry," Abstract #A204, Proceedings of the American Academy of Forensic Sciences, 65th Annual Scientific Meeting, Washington, DC. 2013.

Forensic Toxicology, Methcathinone, Dispersive LLE